

Supplementary Information

Synthesis and antibacterial activities evaluation of C-5 side chain modified analogues of FYL-66, a potential agent against methicillin-resistant *Staphylococcus aureus*

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1. Experimental Data

1.1. Assay for cytotoxicities of compound 40

In cytotoxicity analysis, inhibition ratios were calculated from MTT method on HEK293A cells and L02 cells. The equation of inhibition ratio is as follows: inhibition ratio % = $(A-B)/A \times 100\%$, here, A= OD of control group, B= OD of drug group. Inhibition ratio curves of **40** for HEK293A cells and L02 cells were obtained by GraphPad Prism 5 and shown in figure 1.

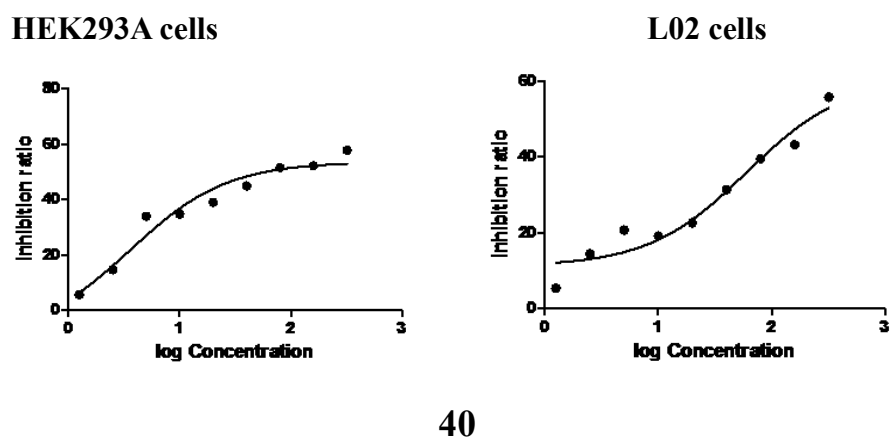


Figure 1. Inhibition ratio curves of **40** for HEK293A cells and L02 cells

1.2. Assay for aqueous solubilities of Linezolid, FYL-66 and compound 40

Calibration curves were obtained by plotting the peak area against the corresponding concentration. And the aqueous solubility Calibration curves for compounds Linezolid, FYL-66 and **40** are in figure 2.

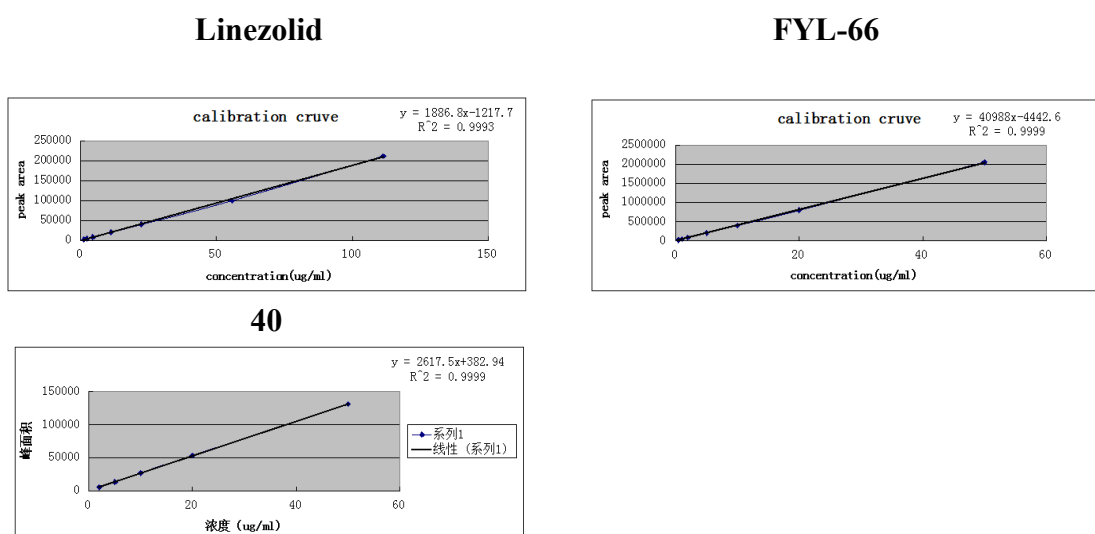
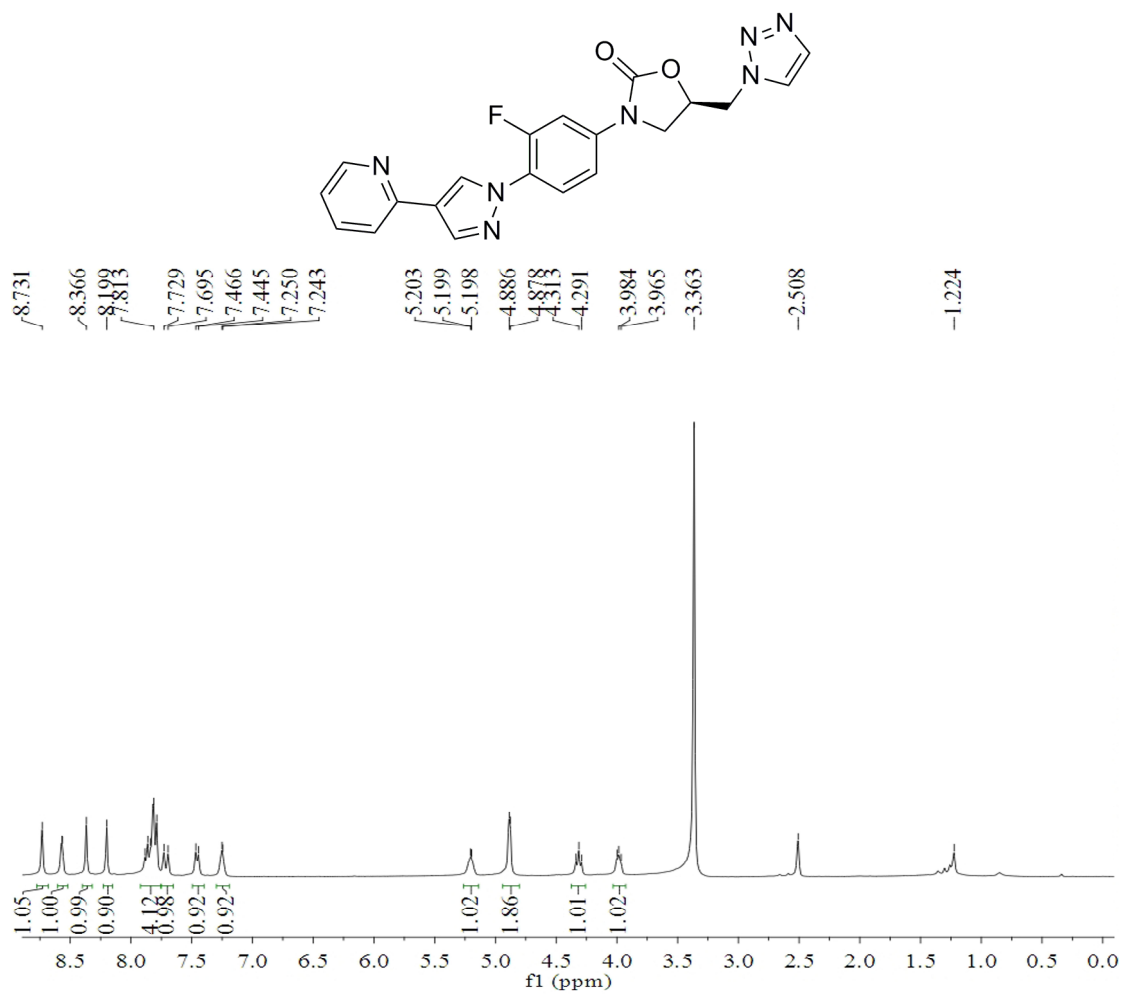
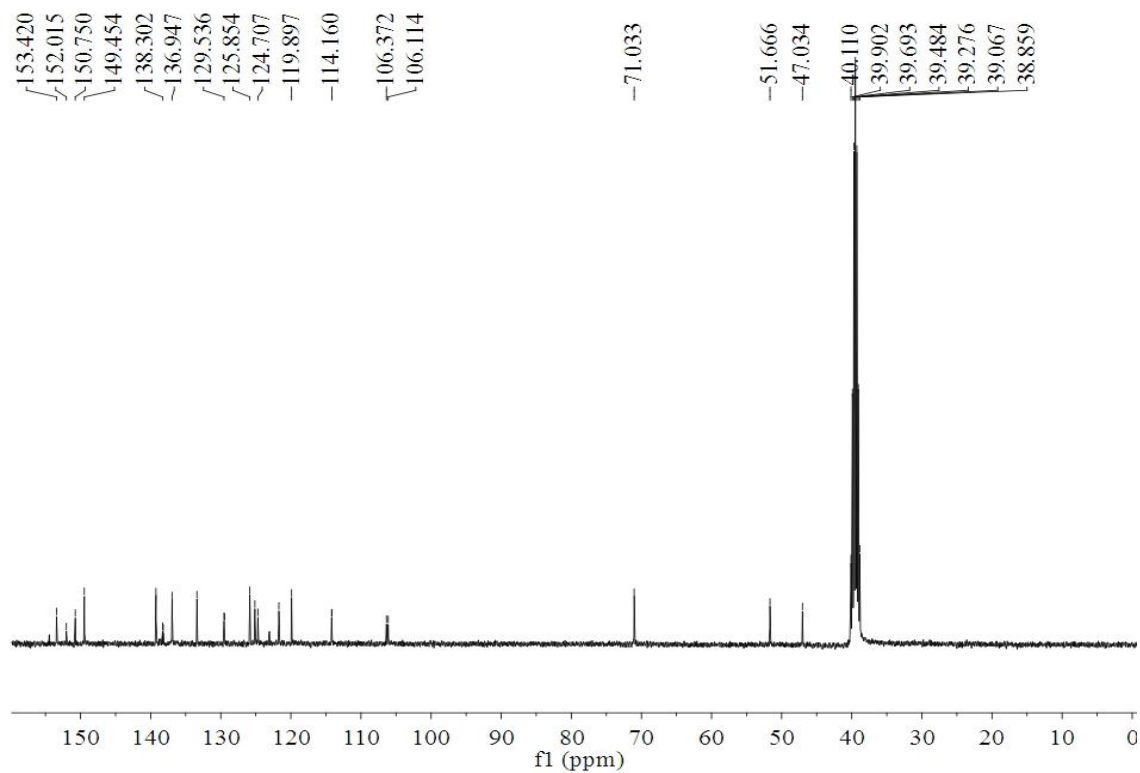


Figure 2. Aqueous solubility calibration curves of Linezolid, FYL-66 and **40**

1.3. ^1H , ^{13}C NMR, MS and HRMS of compounds 31, 33, 34, 37-40 and 43-45

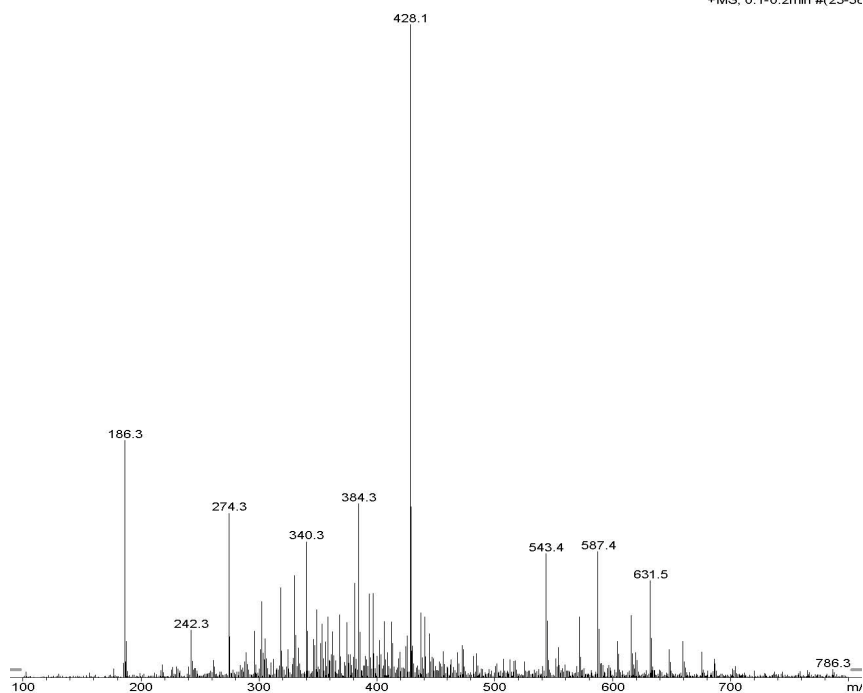
Compounds 31





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+MS, 0.1-0.2min # (23-36)



mpass DataAnalysis 4.0

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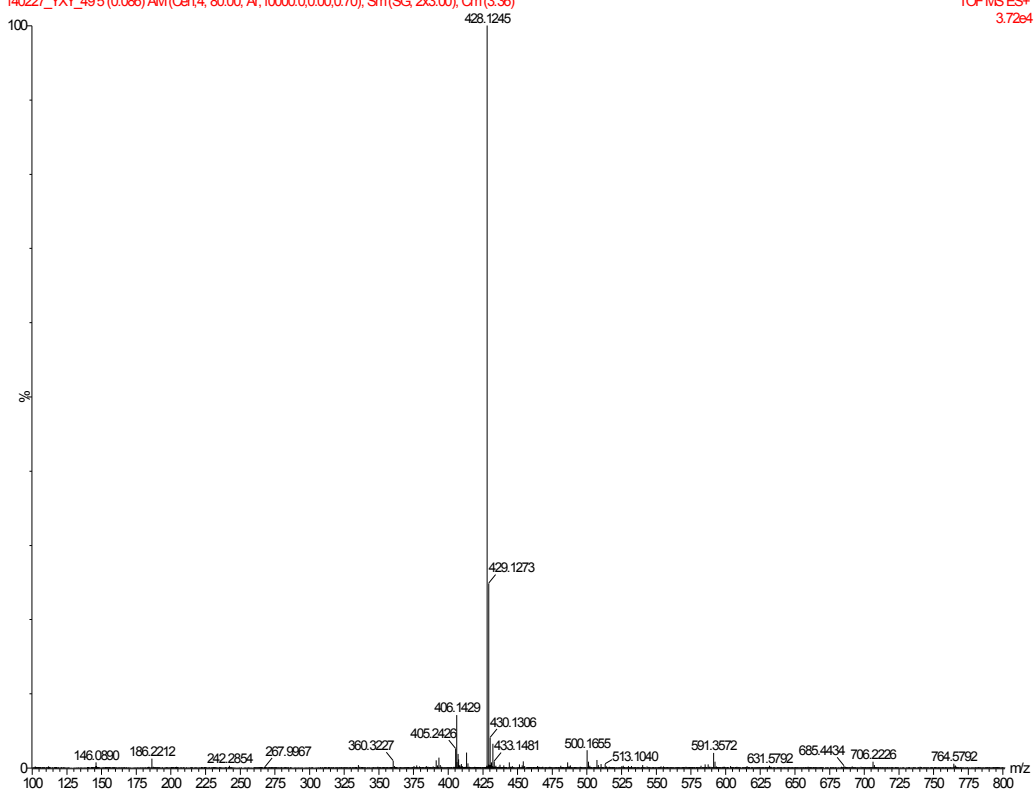
Page 1 of 1

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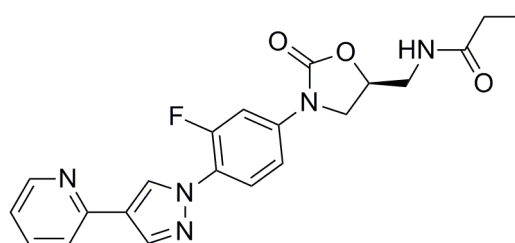
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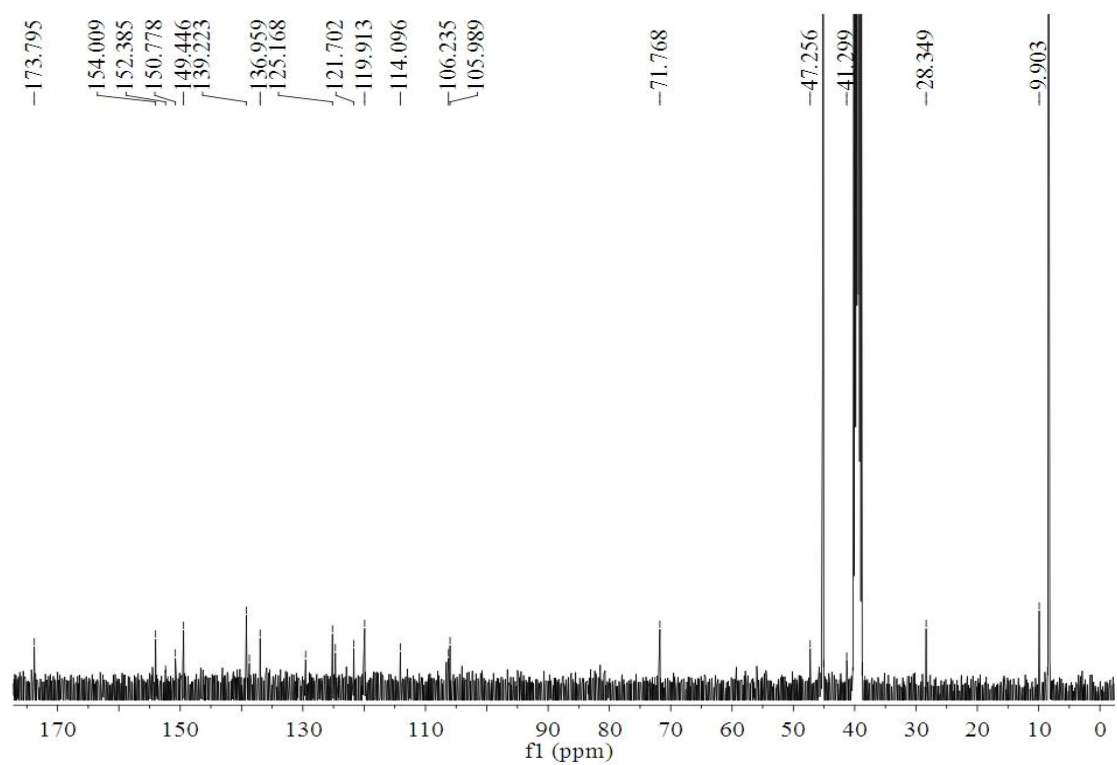
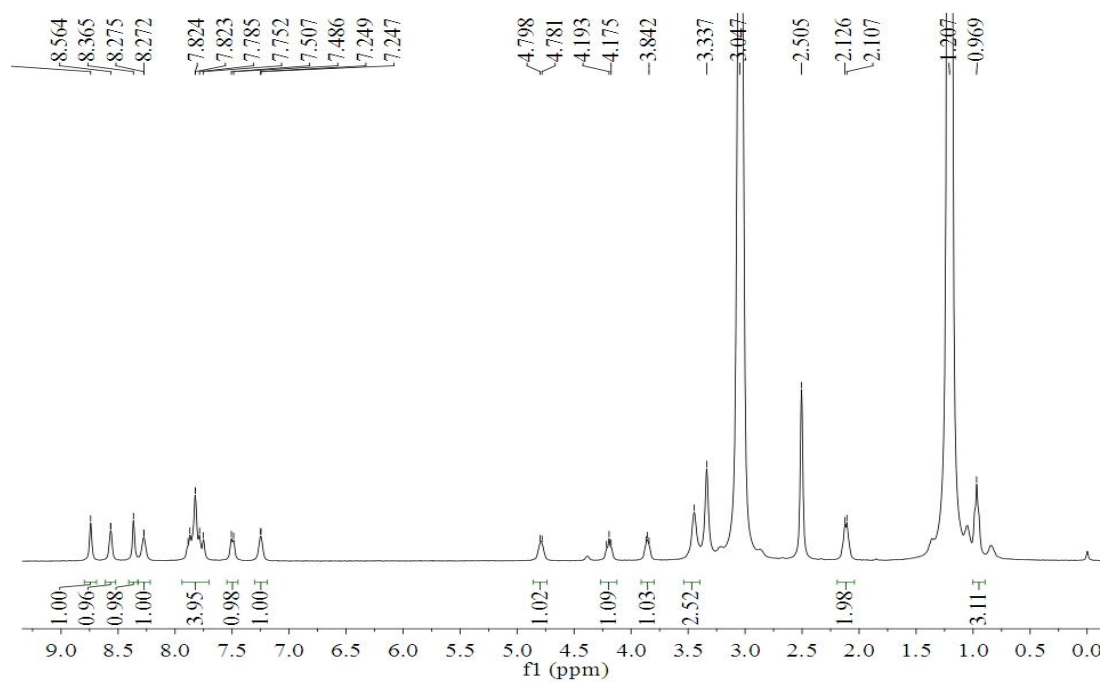
27-Feb-2014

TOF MS ES+
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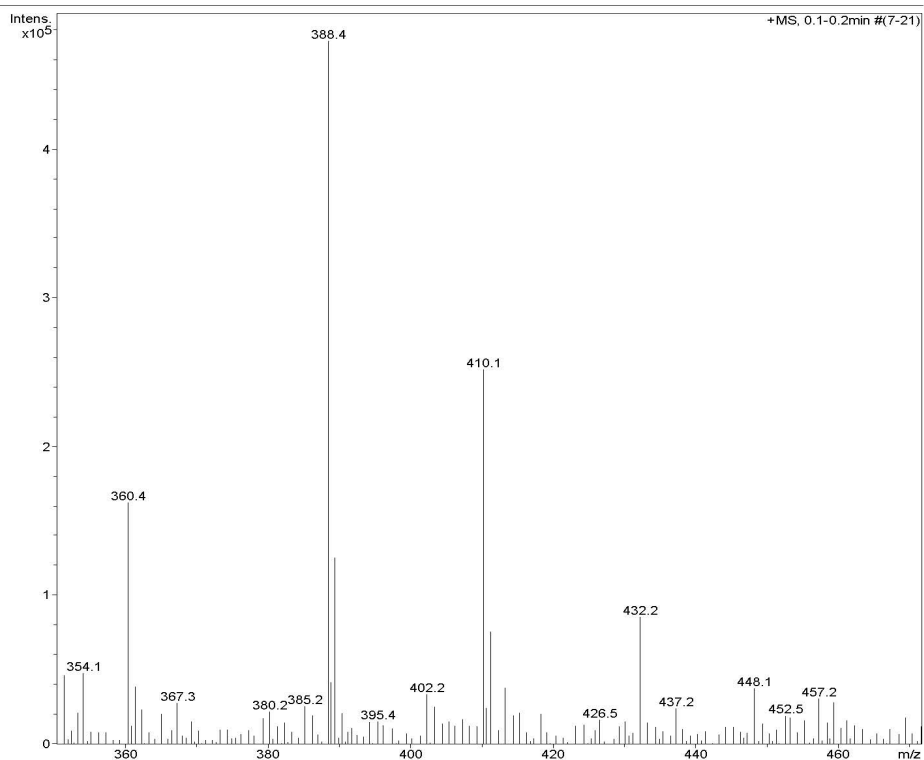
Compounds 33





Acquisition Parameter

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Capillary Exit	140.0 V	n/a	n/a	Trap Drive	53.6
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Bruker Compass DataAnalysis 4.0

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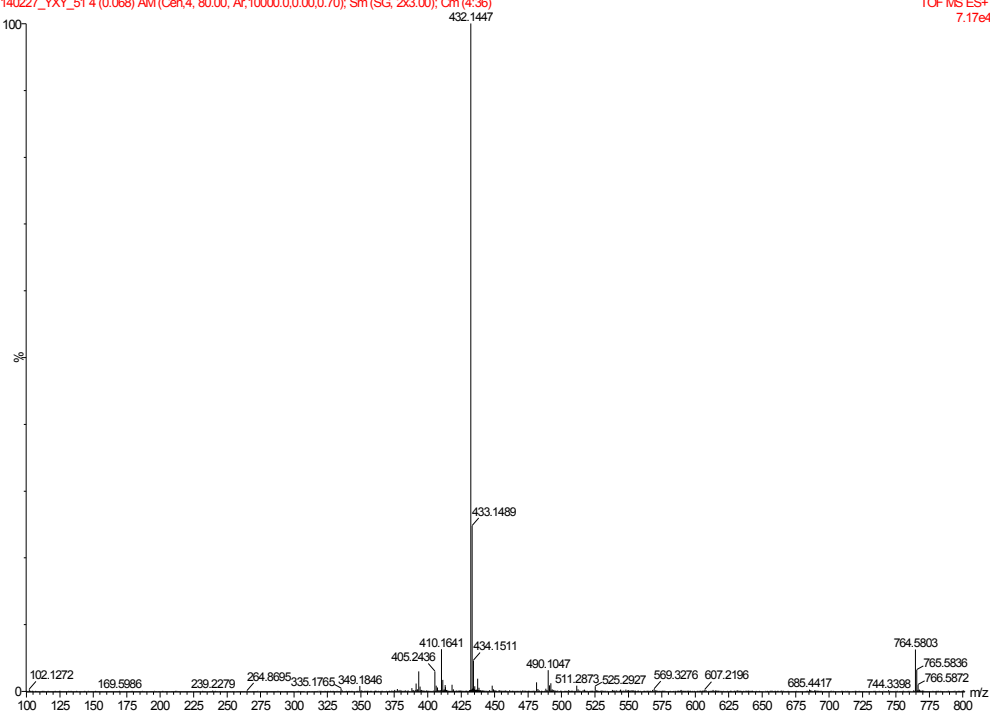
Page 1 of 1

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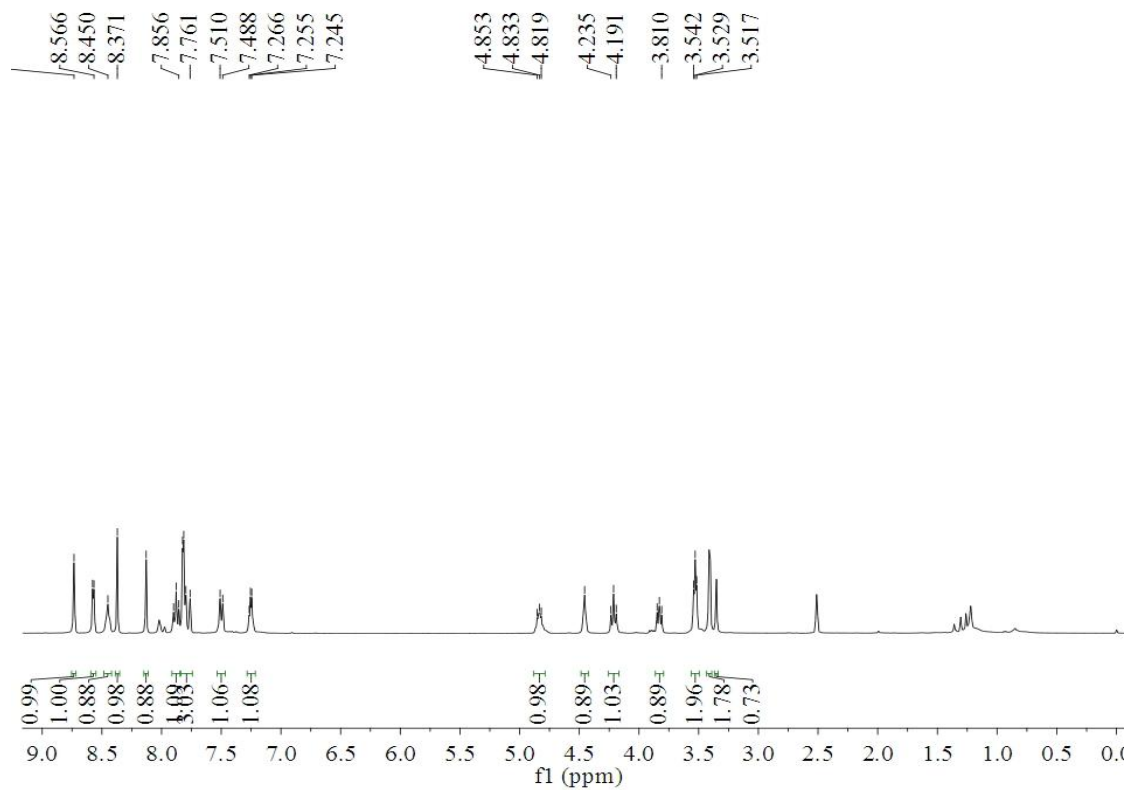
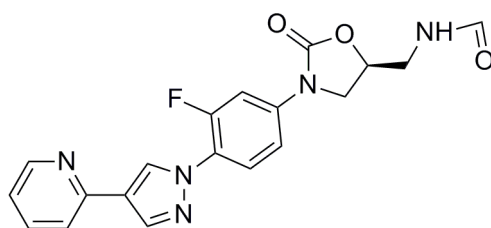
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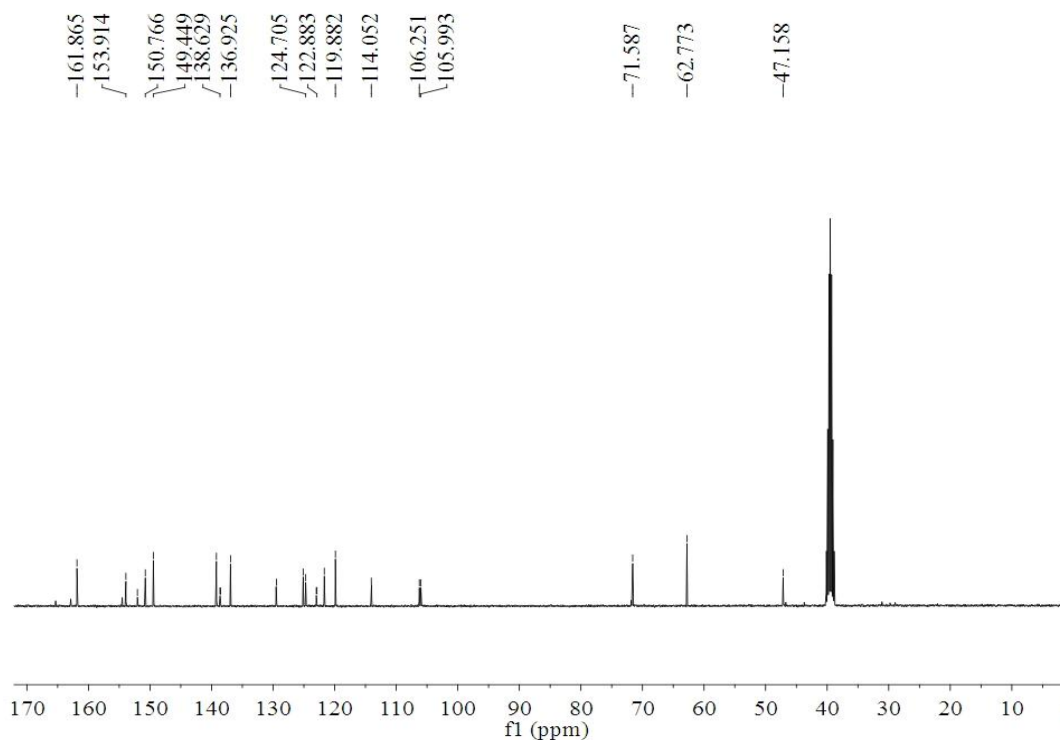
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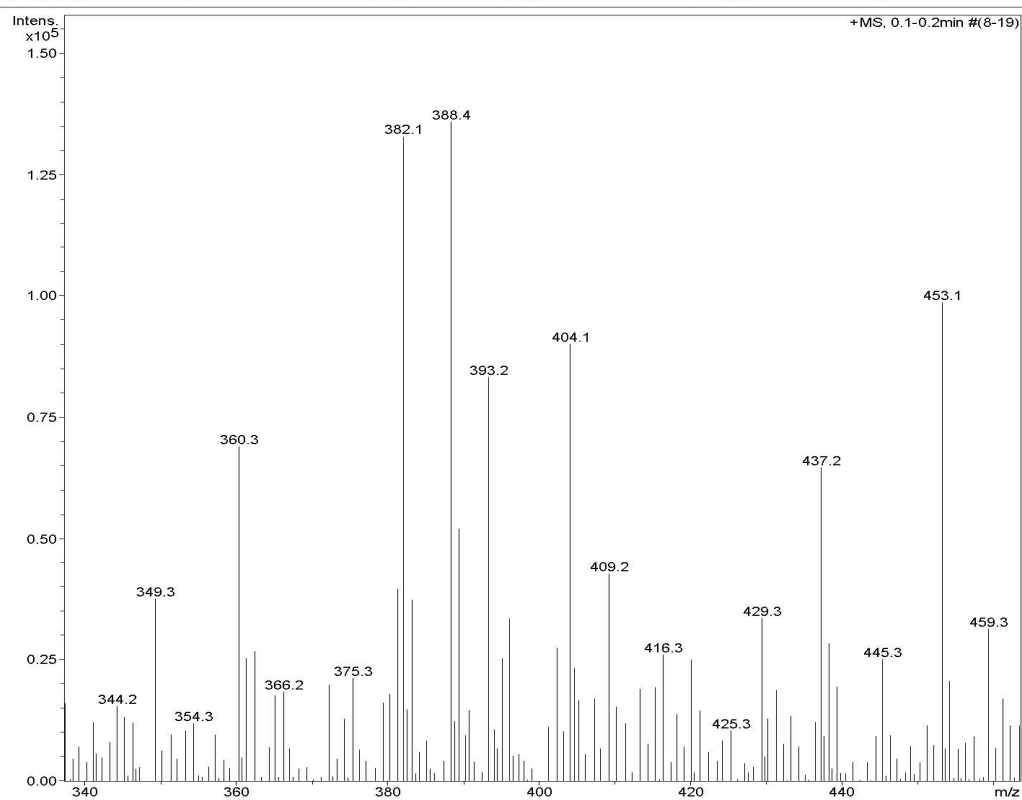
Compounds 34





Acquisition Parameter

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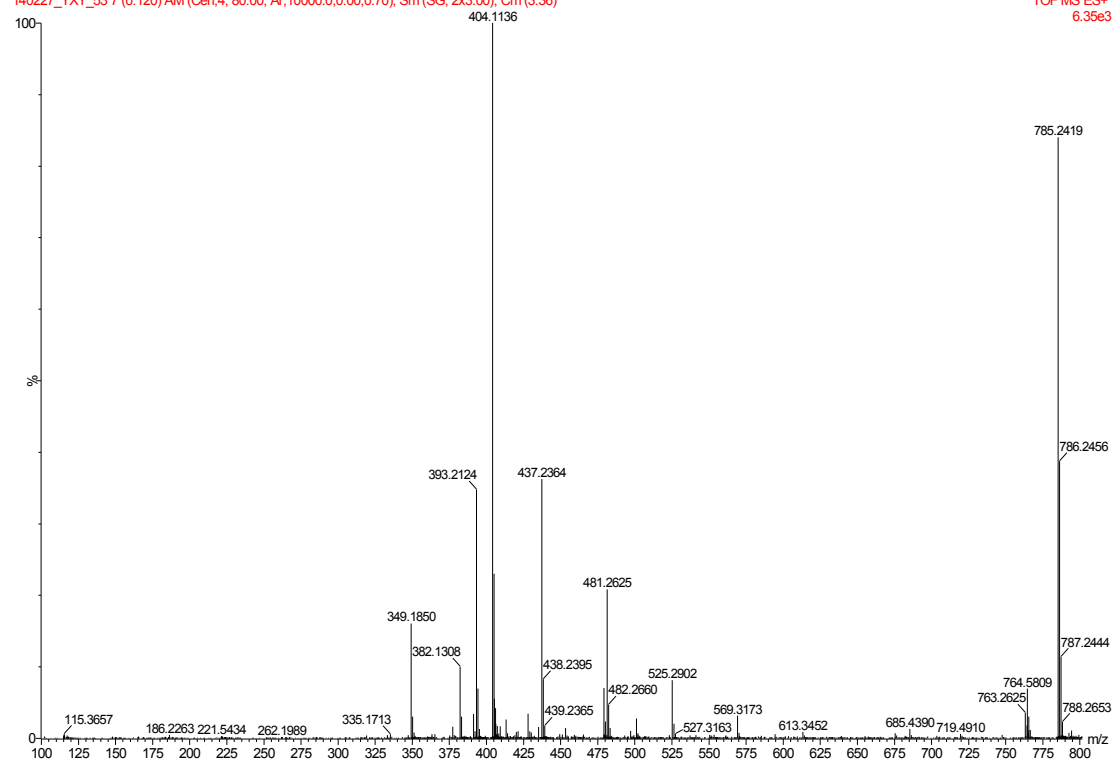


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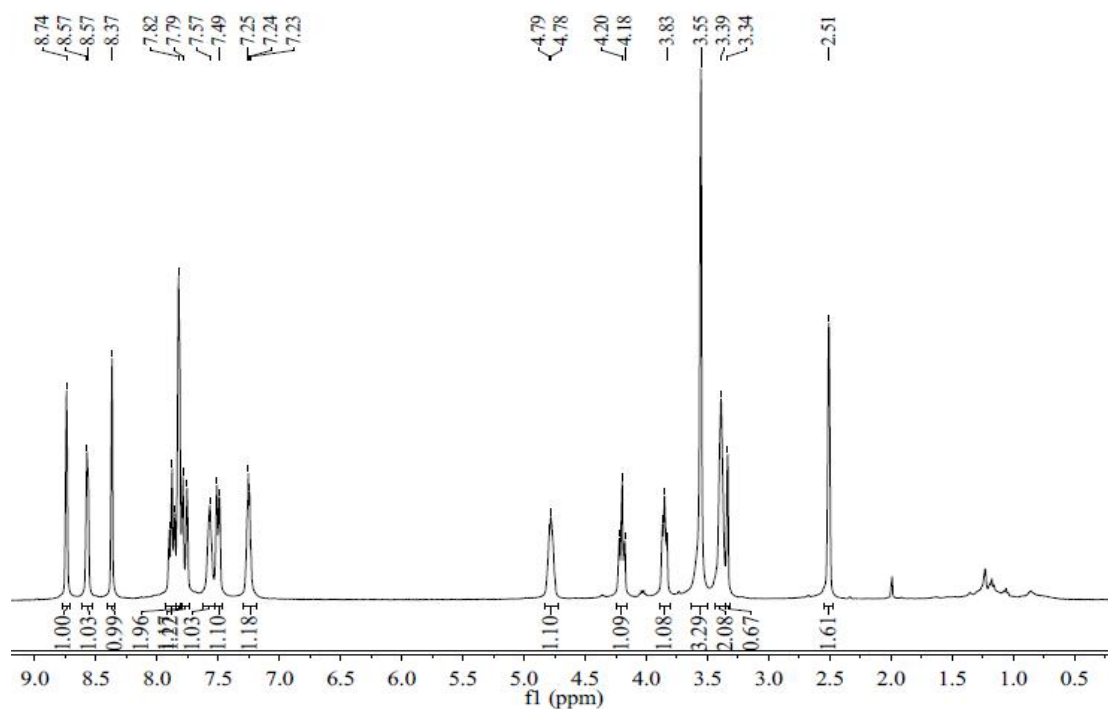
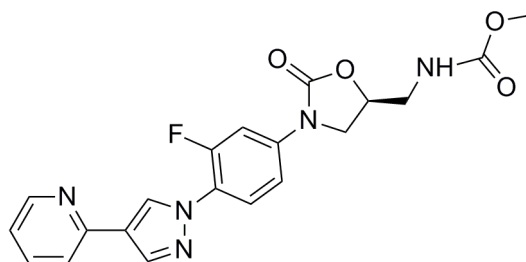
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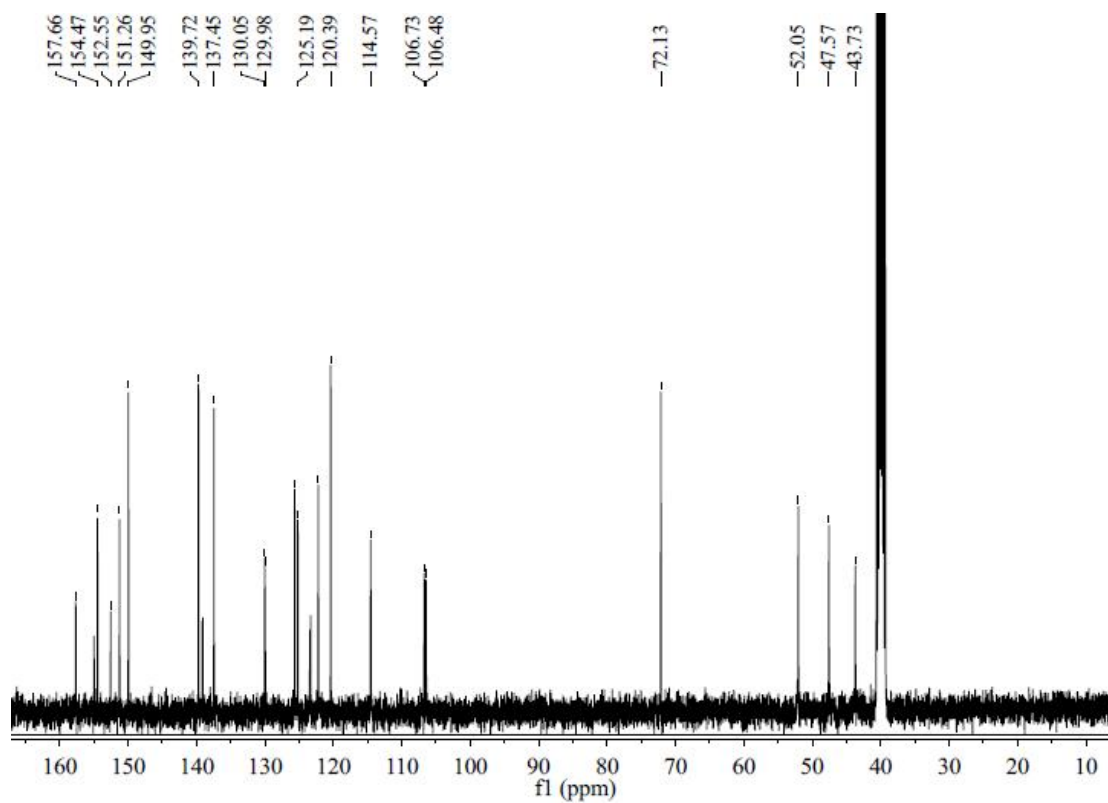
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TOF MS ES+
6.35e3



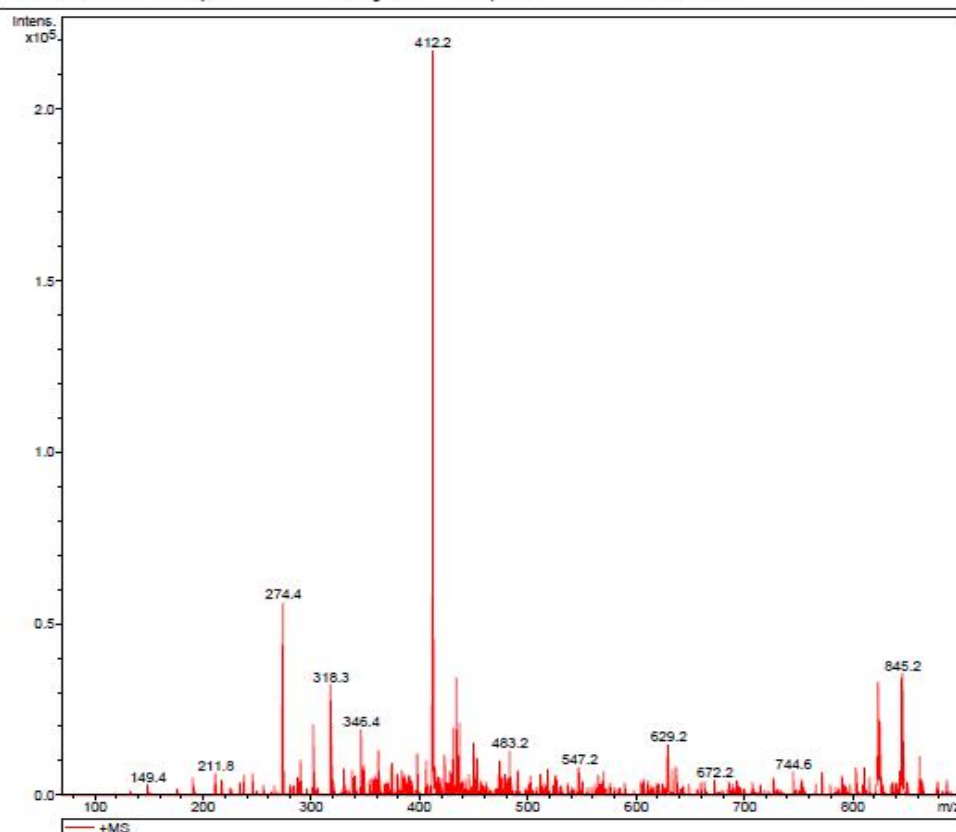
Compounds 37





Acquisition Parameter

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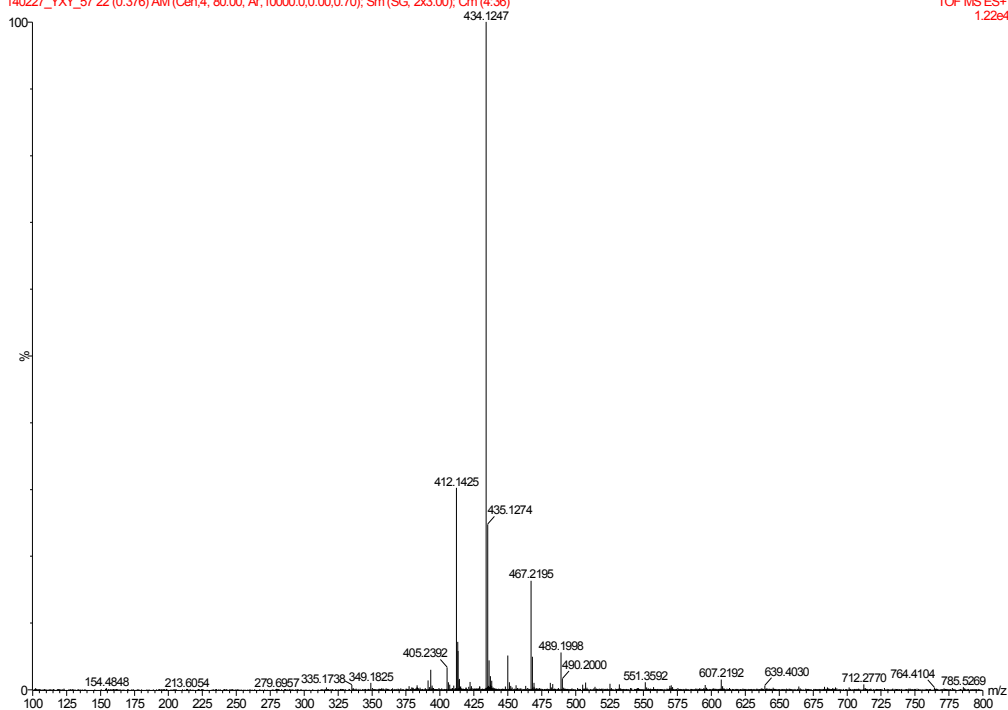


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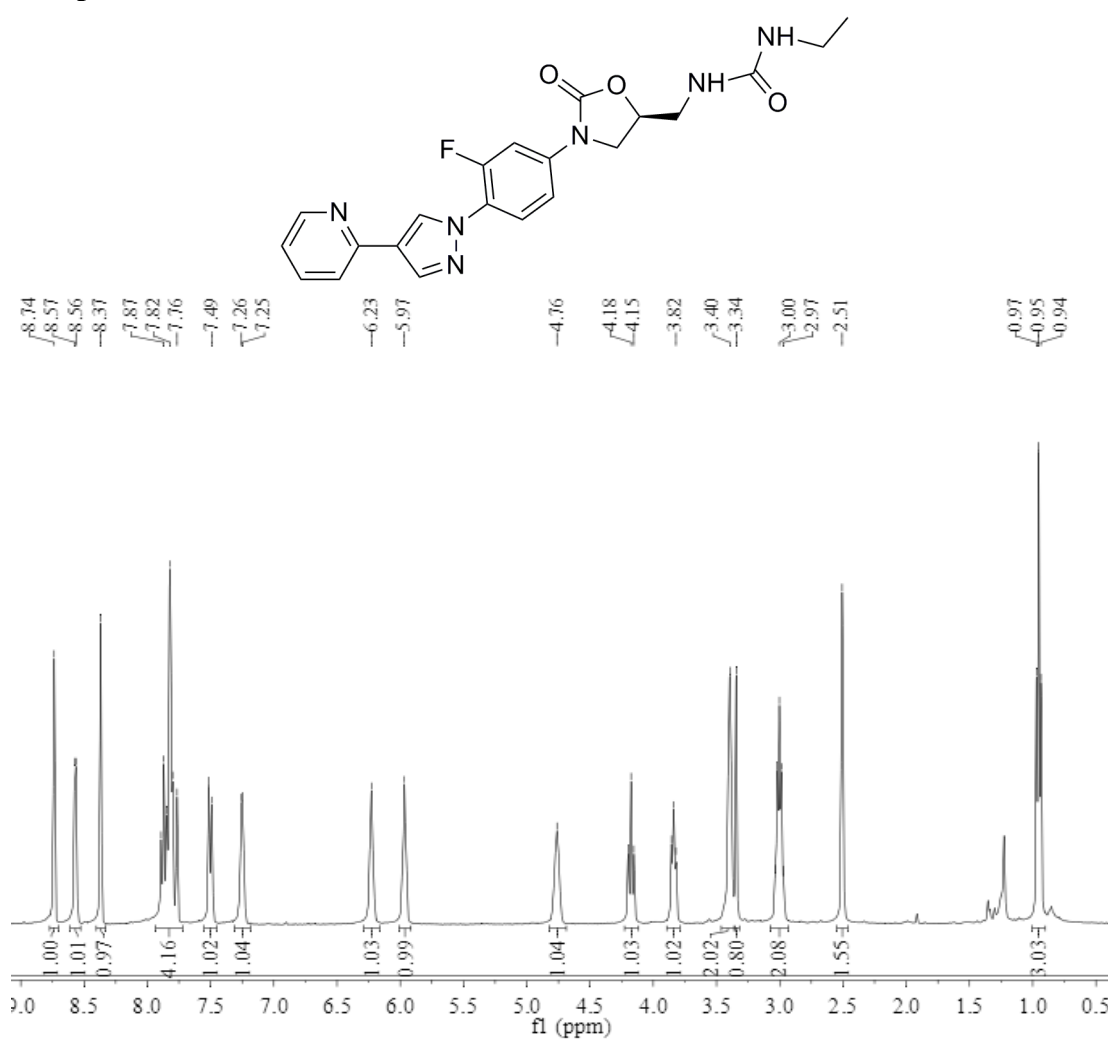
140227_YXY_57 22 (0.376) AM (Cen.4, 80.00, Ar,10000.0,0.00,0.70); Sm (SG, 2x3.00); Cm (4:36)

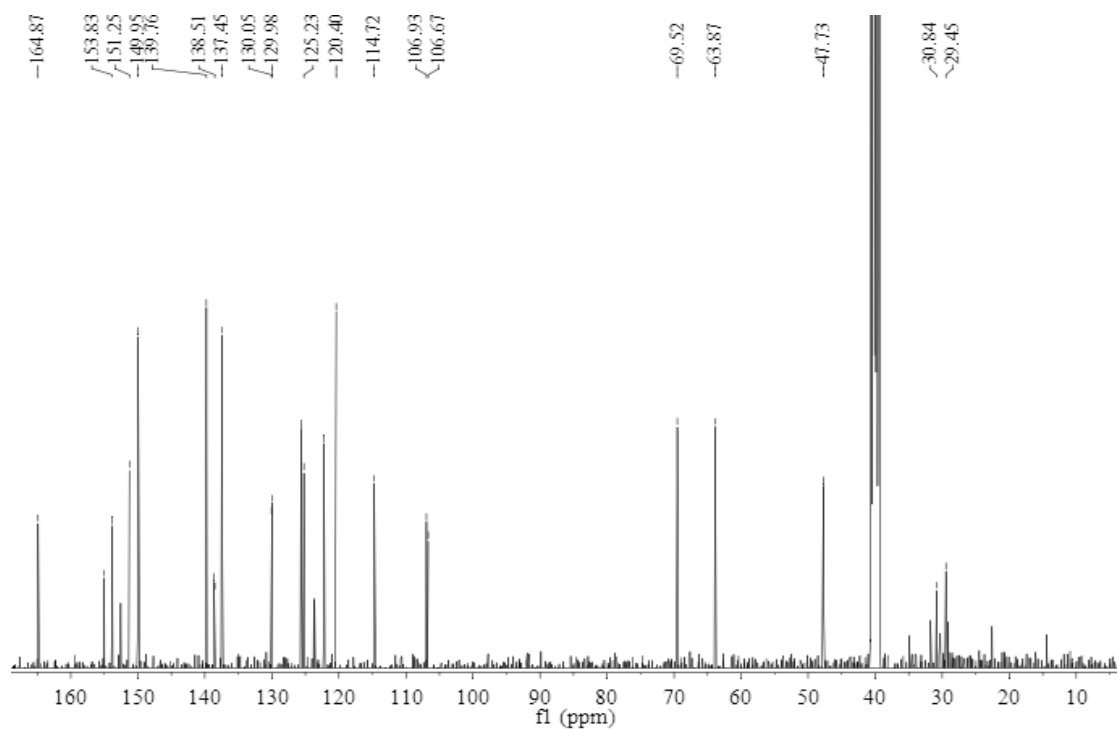
27-Feb-2014

TOF MS ES+
1.22e4



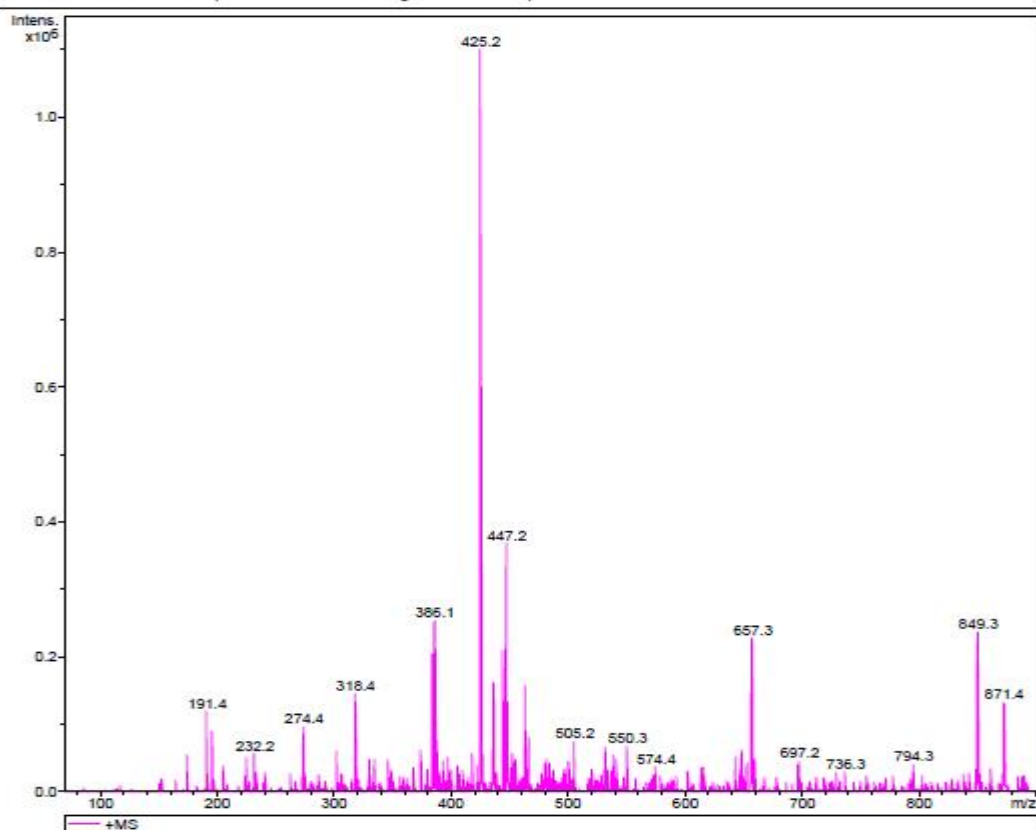
Compounds 38





Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
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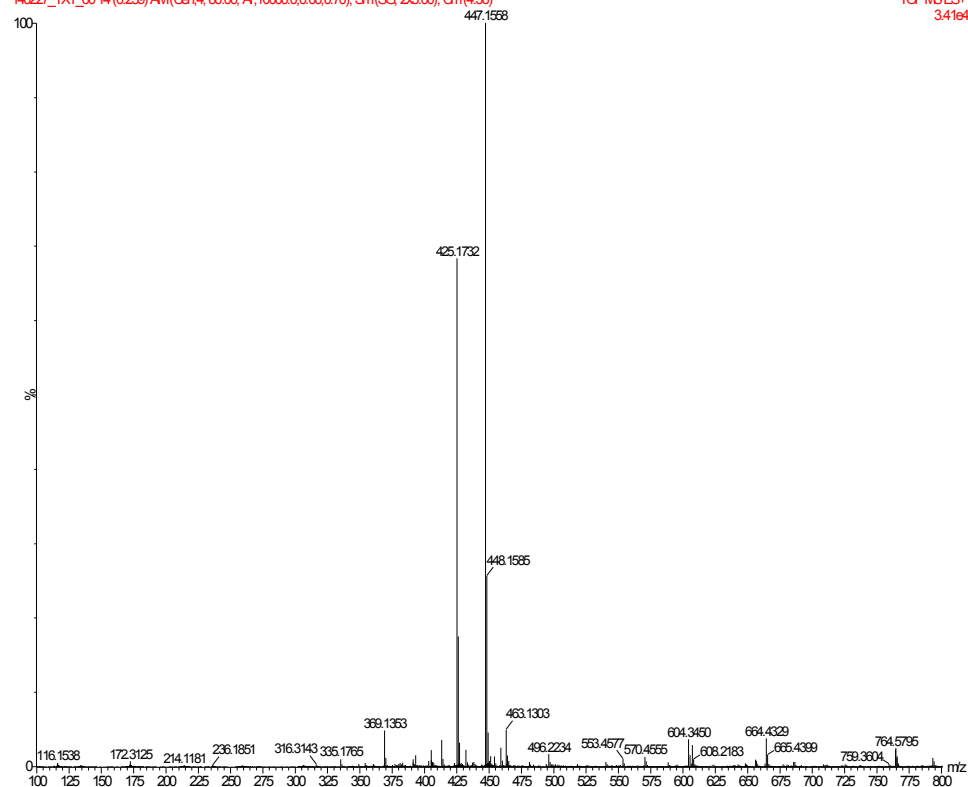


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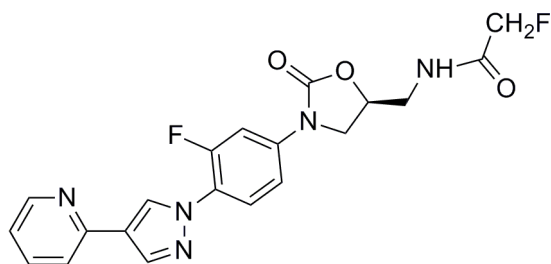
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27-Feb-2014

TOF MS ES+
3.41e4



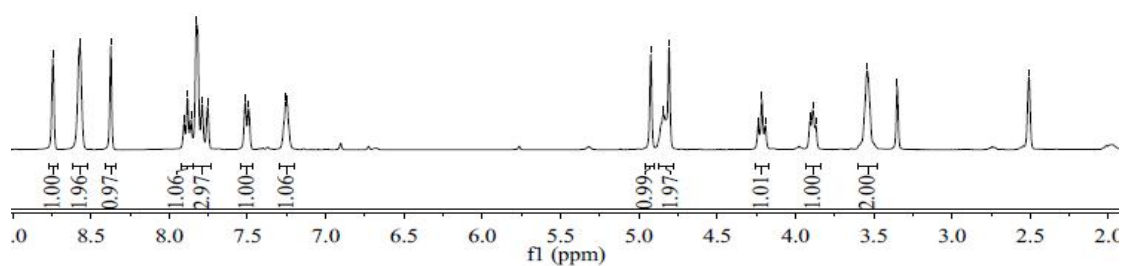
Compounds 39

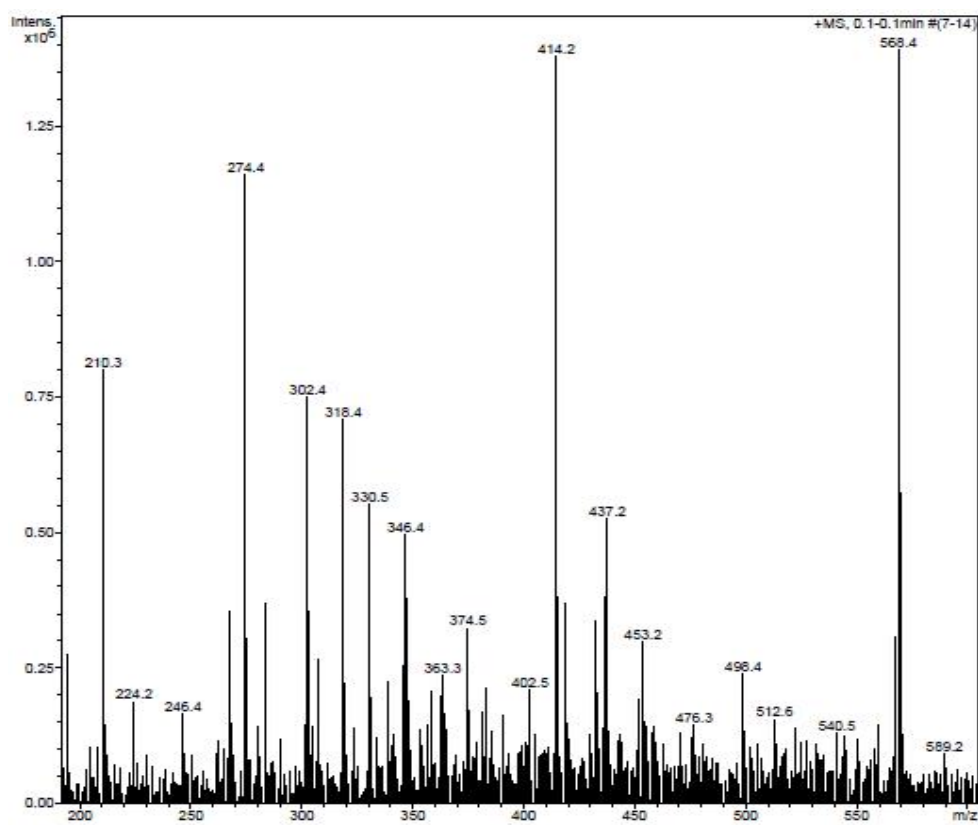
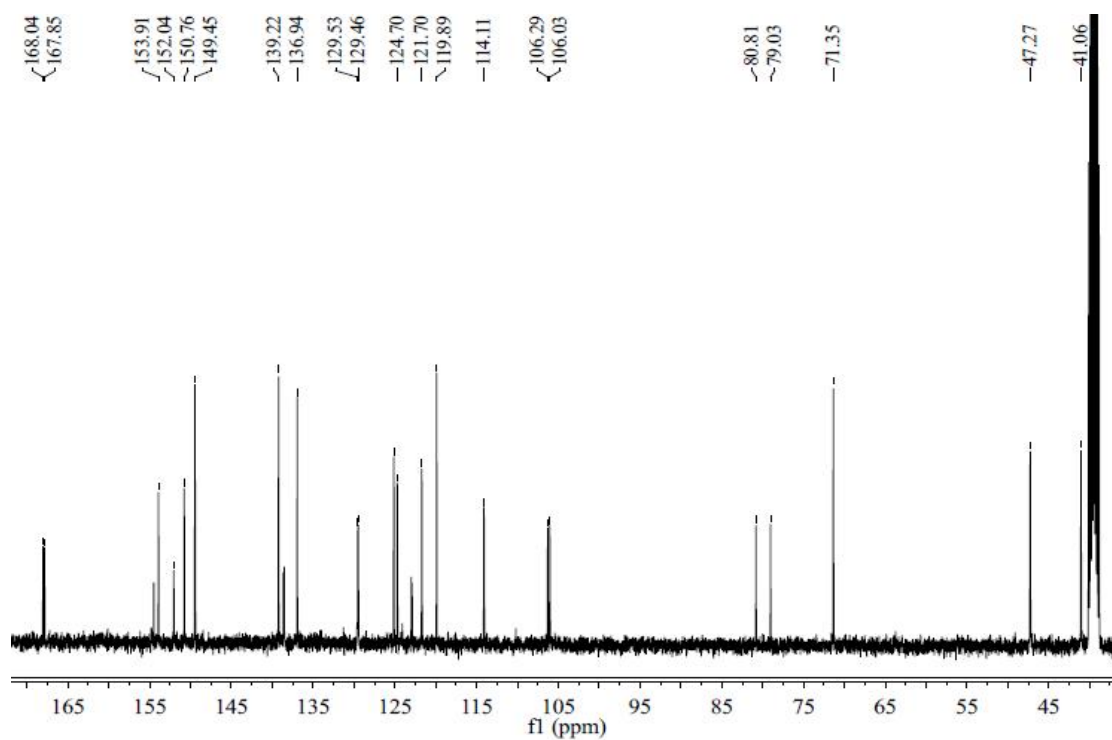


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7.86
7.82
7.75
7.49
7.25
7.25

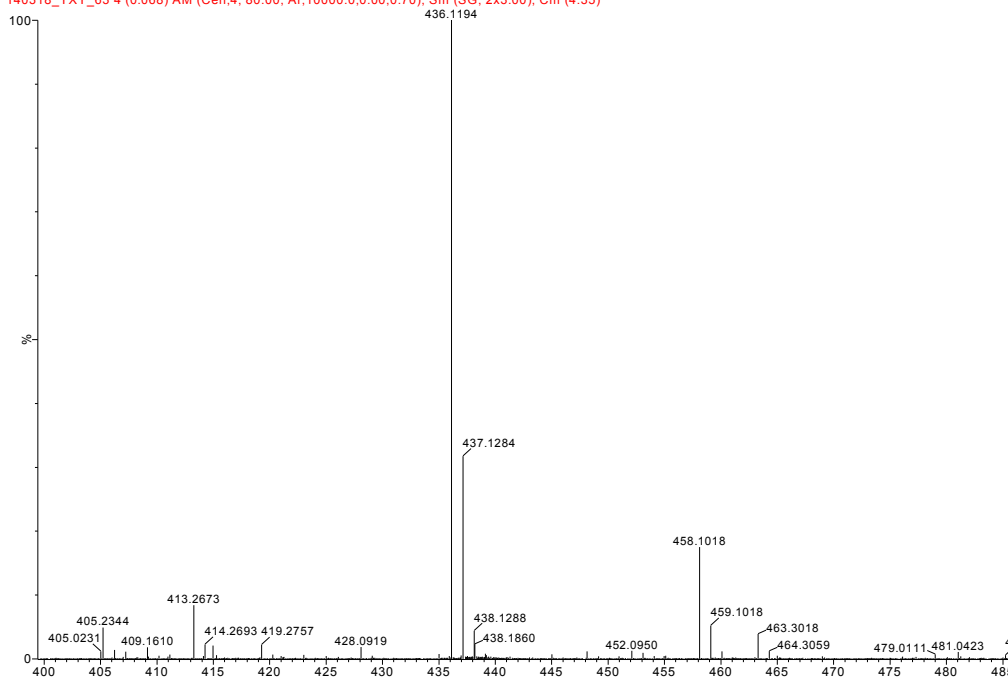
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4.19
3.89
3.87
3.54
3.35

-2.51

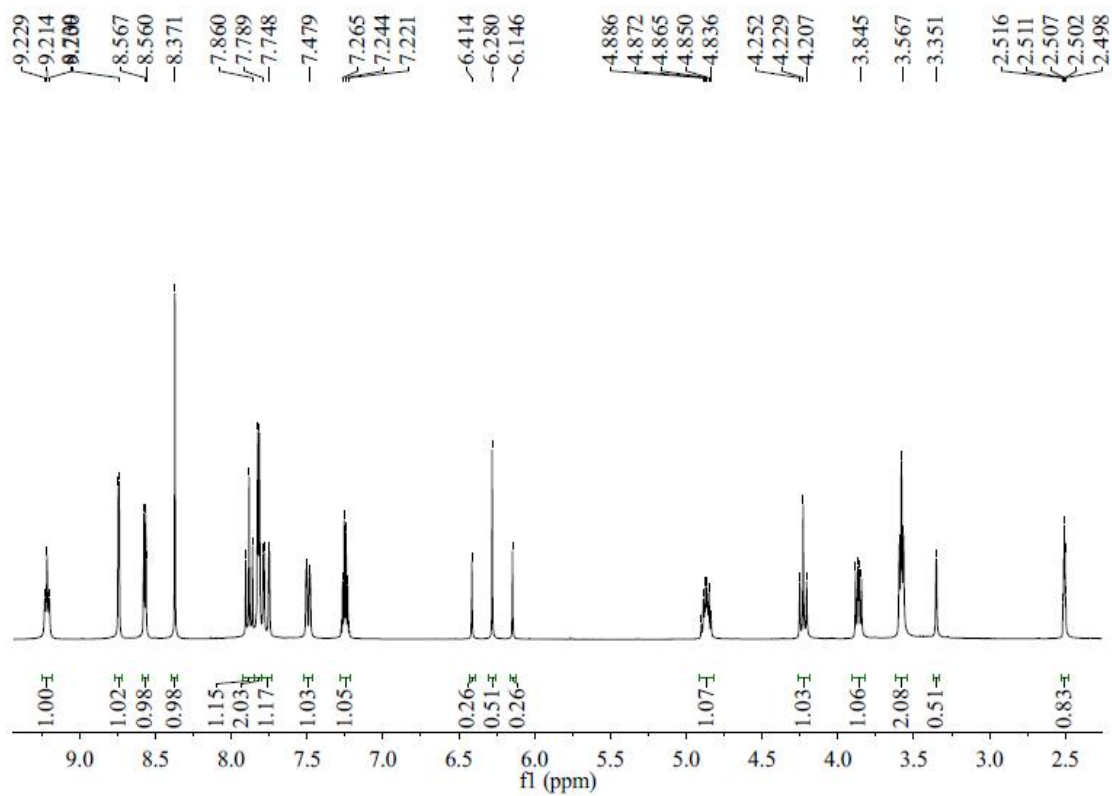
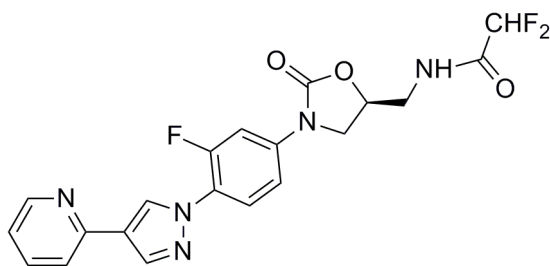


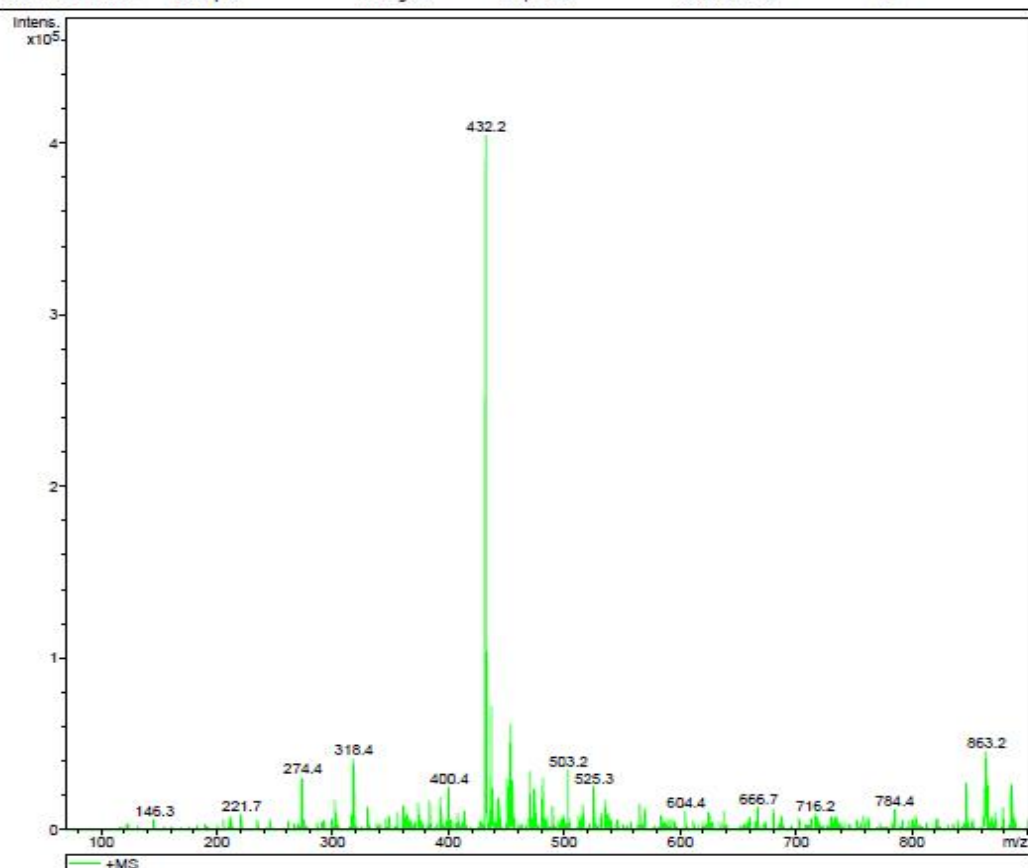
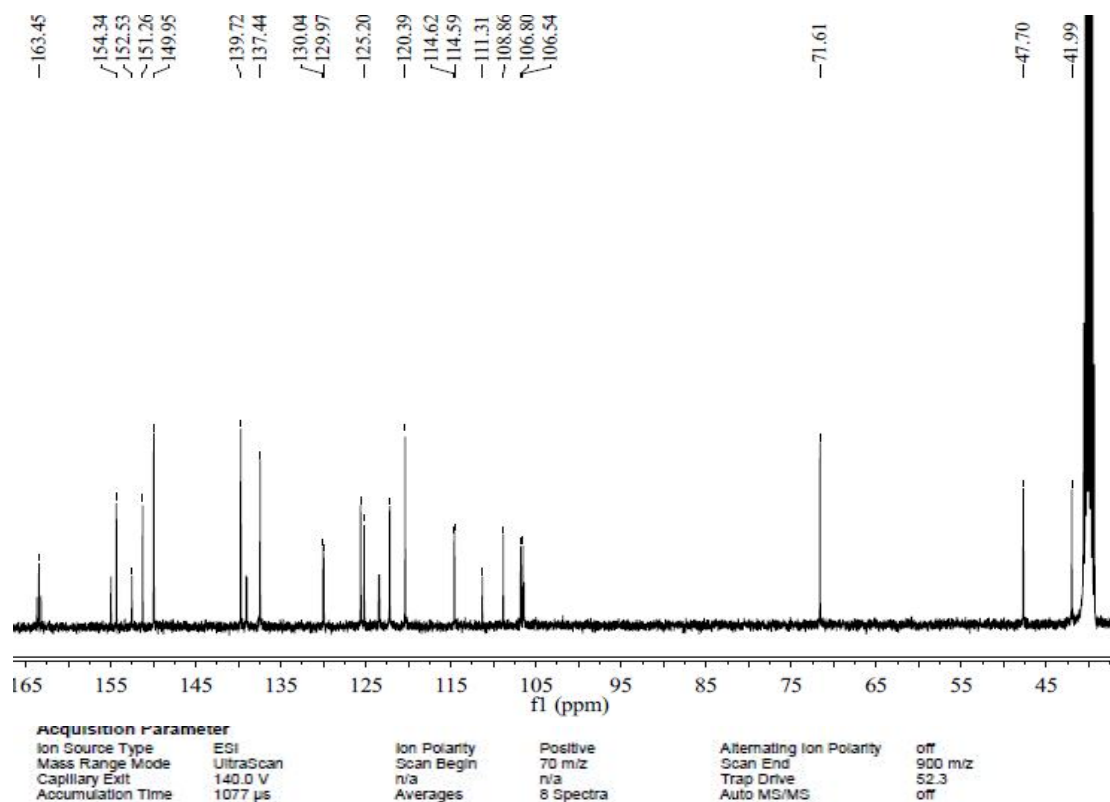


20:02:02
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Compounds 40

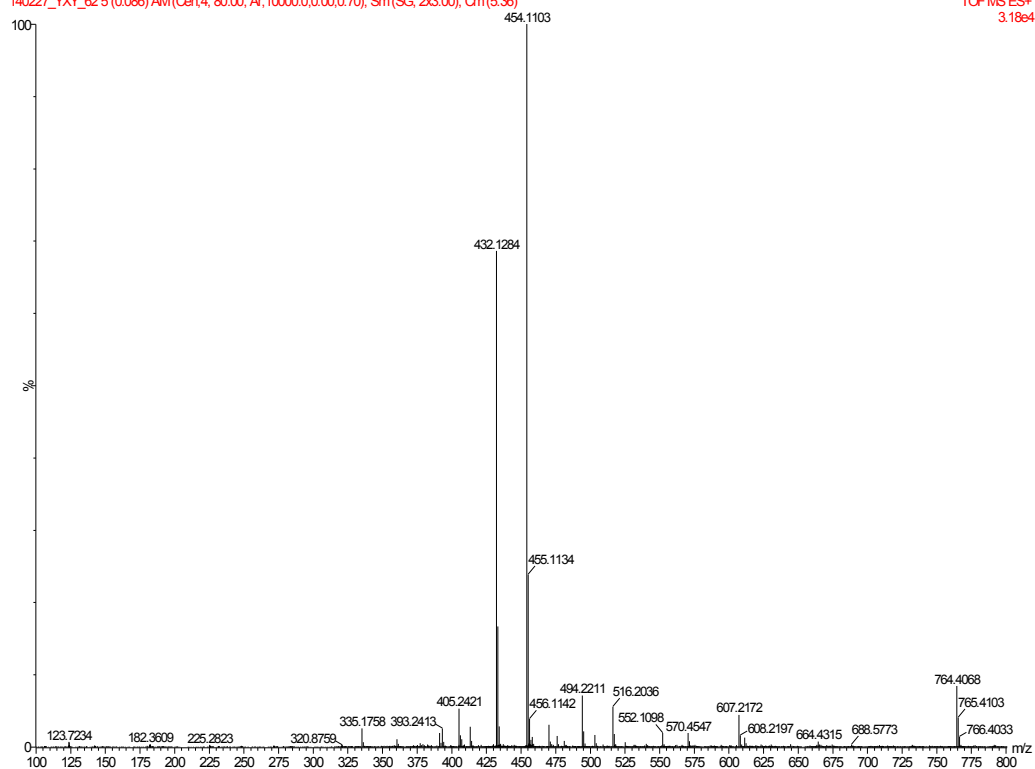
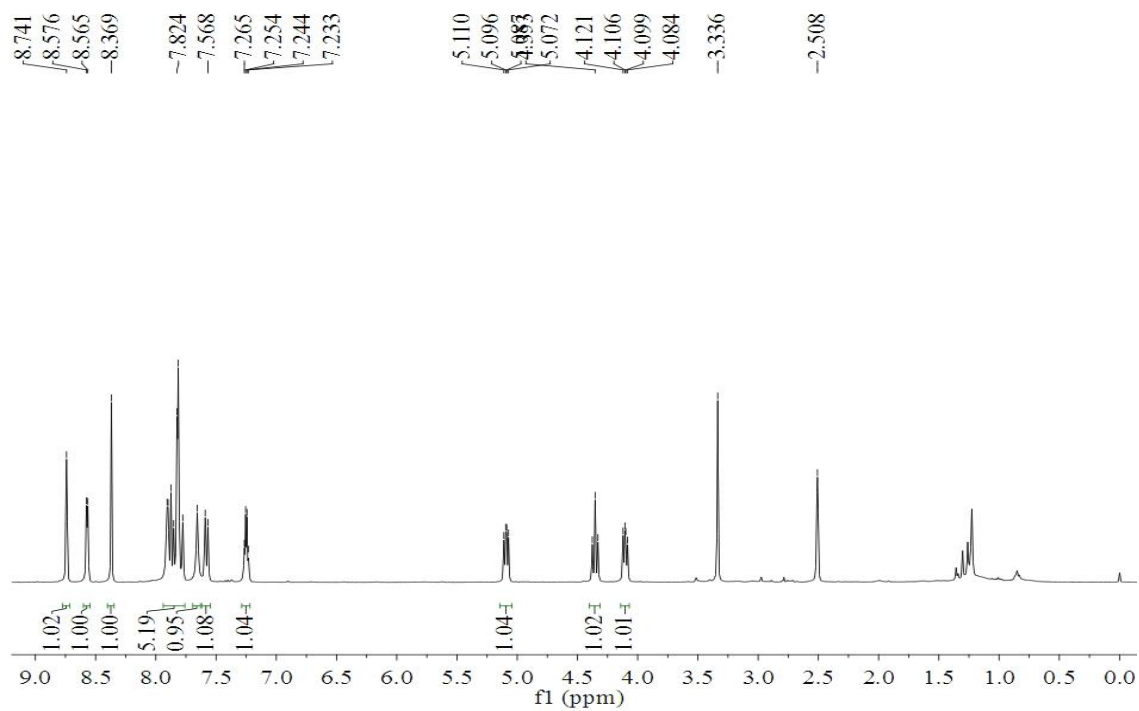


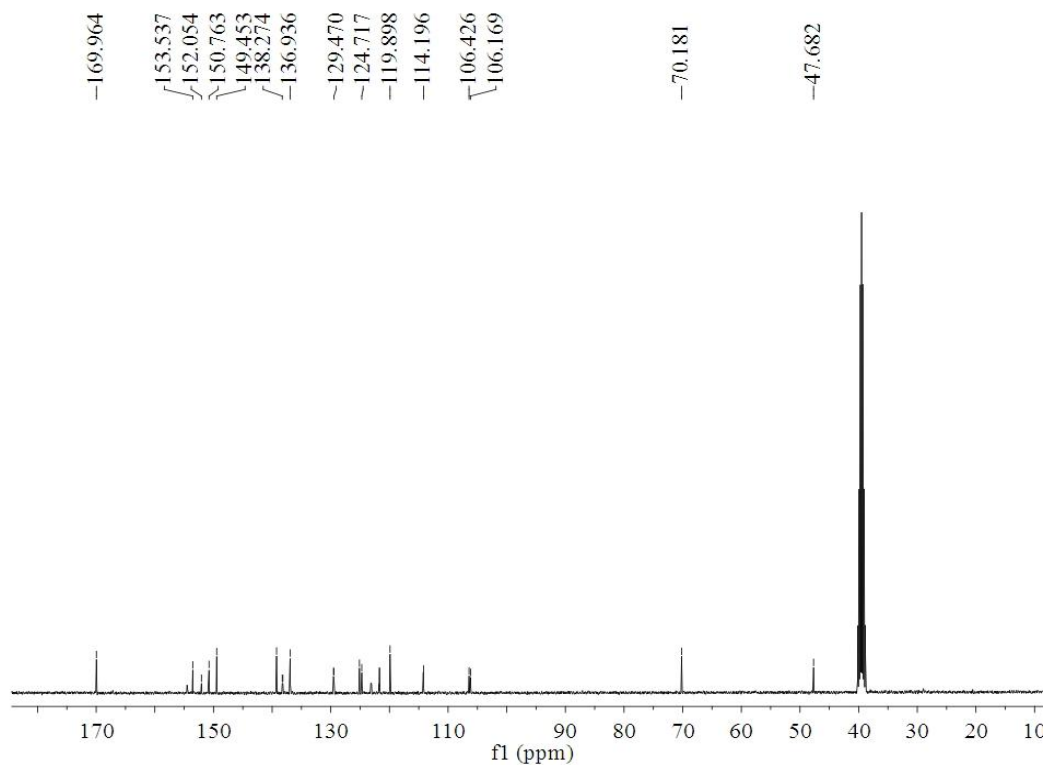


140227 YXY 62 5 (0.086) AM (Cen,4, 80.00, Ar,10000.0,0.00,0.70); Sm (SG, 2x3.00); Cm (5:36)

TOF MS ES+

TOF MS ES+
3.18e4

NC(=O)[C@H]1CN(C(=O)O1)c2cc(F)cc(N3C=CC4=CC=CC=C4N3)c2

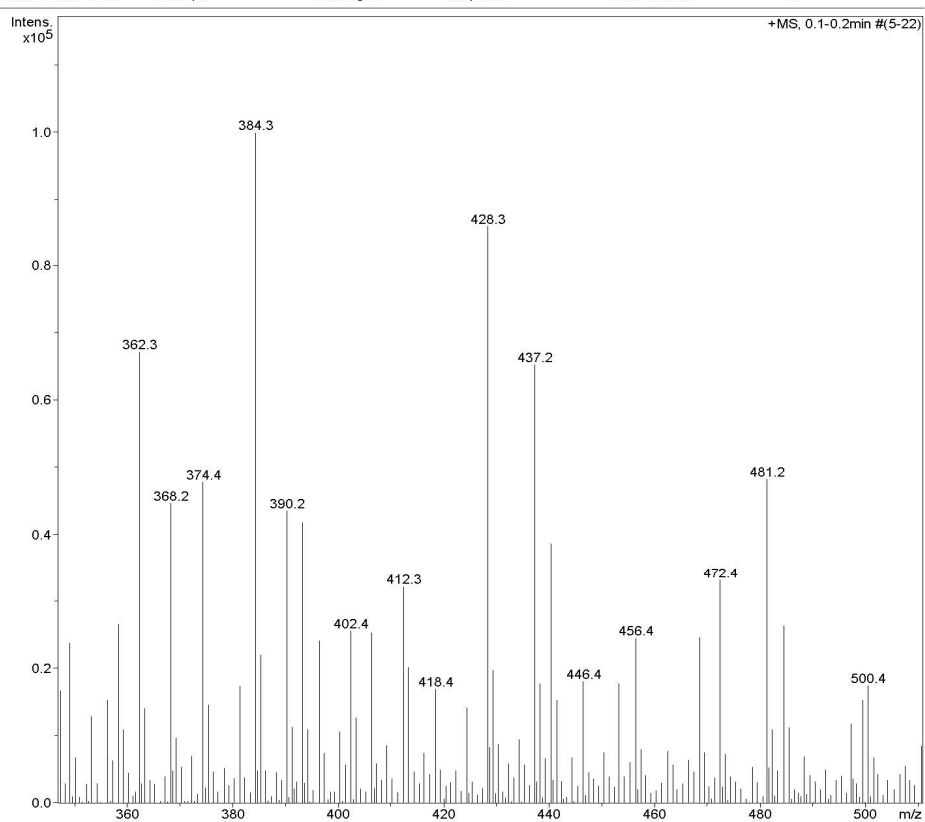


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Averages 8 Spectra

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Auto MS/MS off

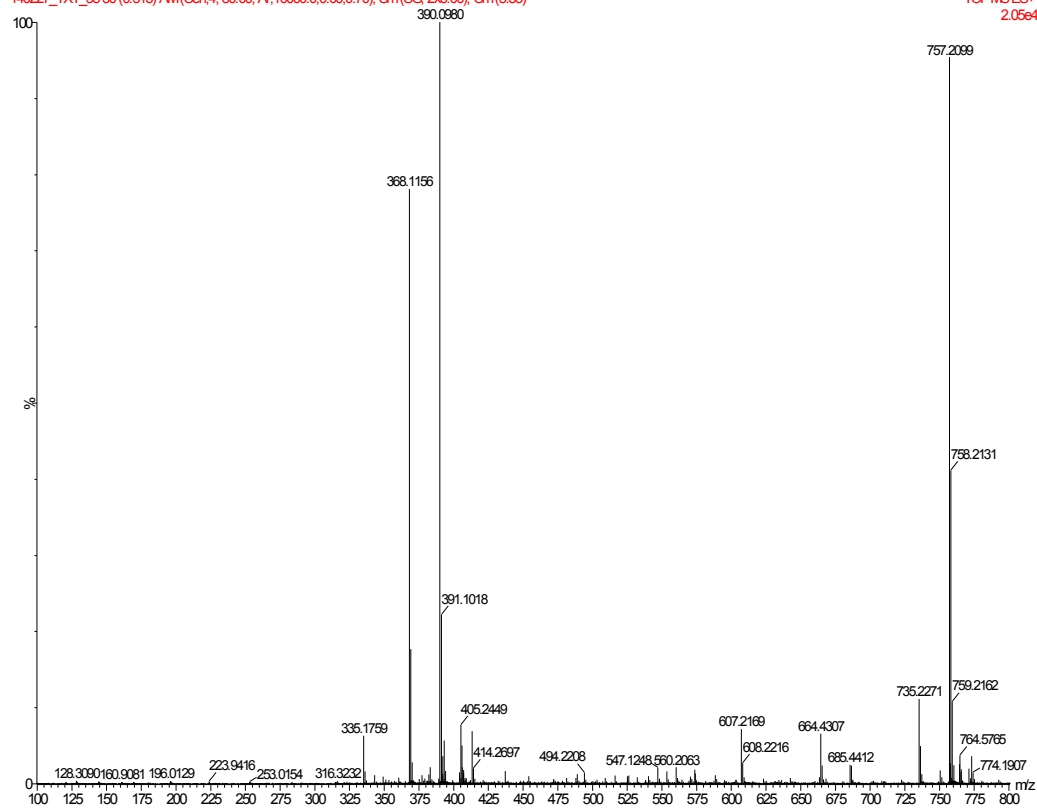


10:17:12

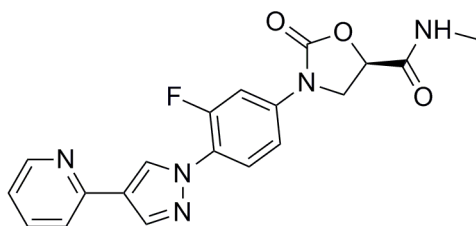
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27-Feb-2014

TOF MS ES+
2.06e4

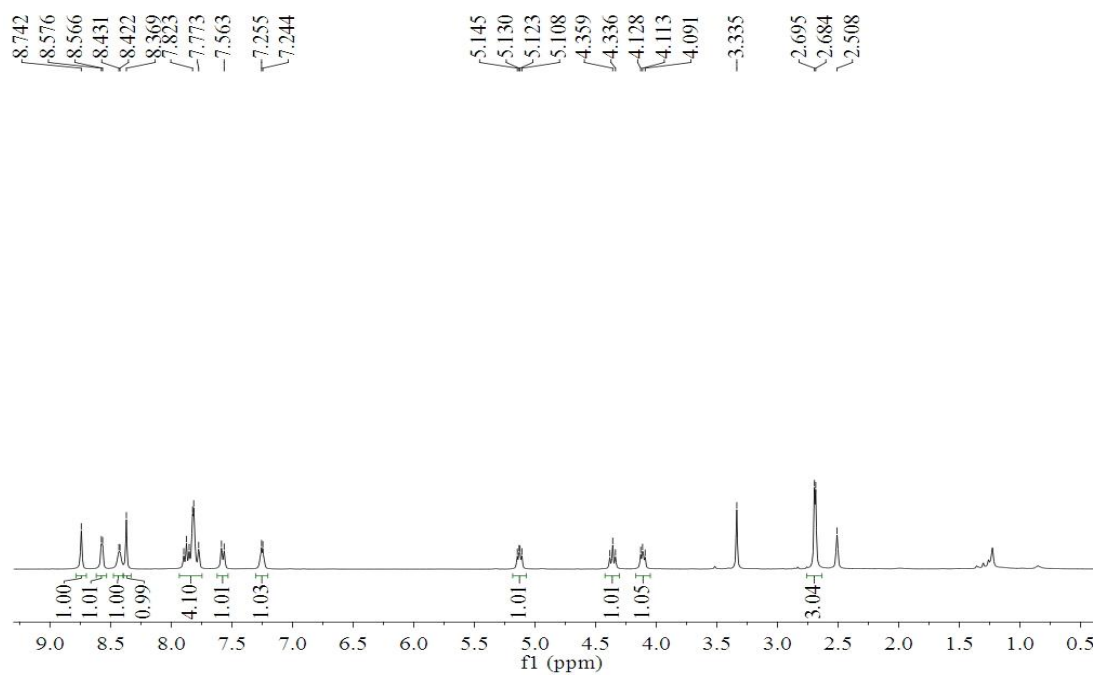


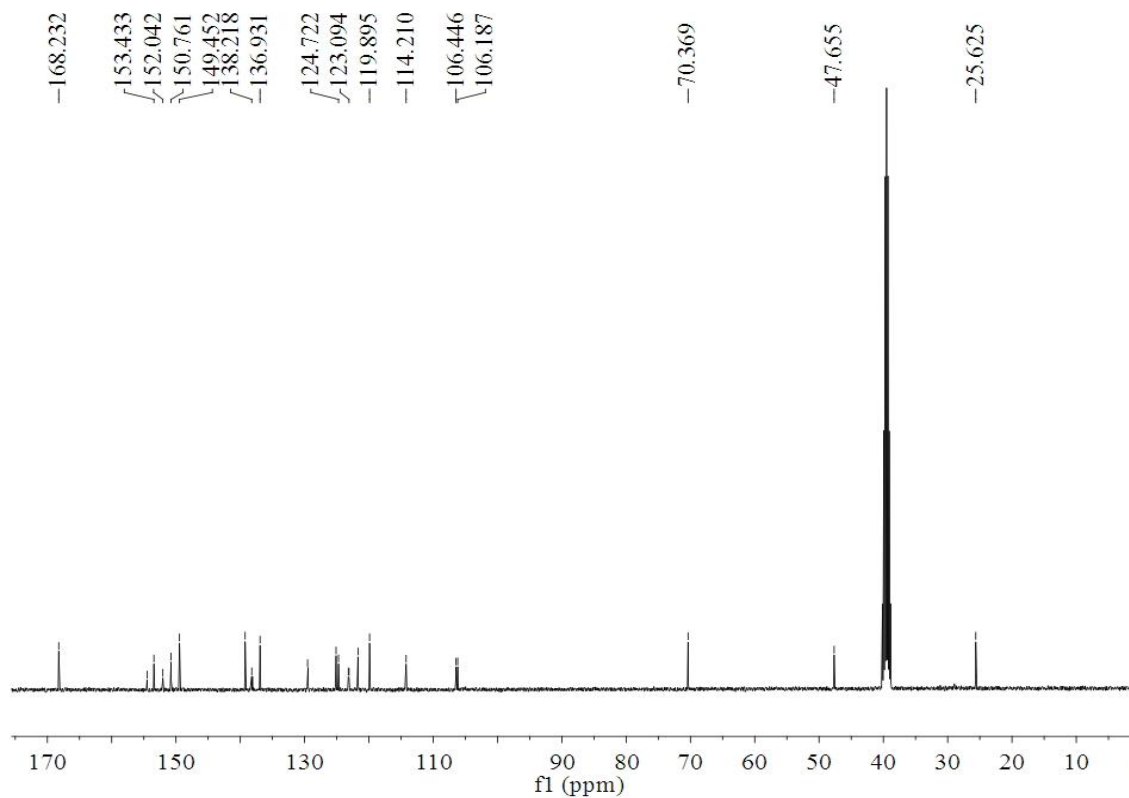
Compounds 44



8.742
8.576
8.566
8.431
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8.369
7.825
7.773
7.563
7.255
7.244

5.145
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2.695
2.684
2.508





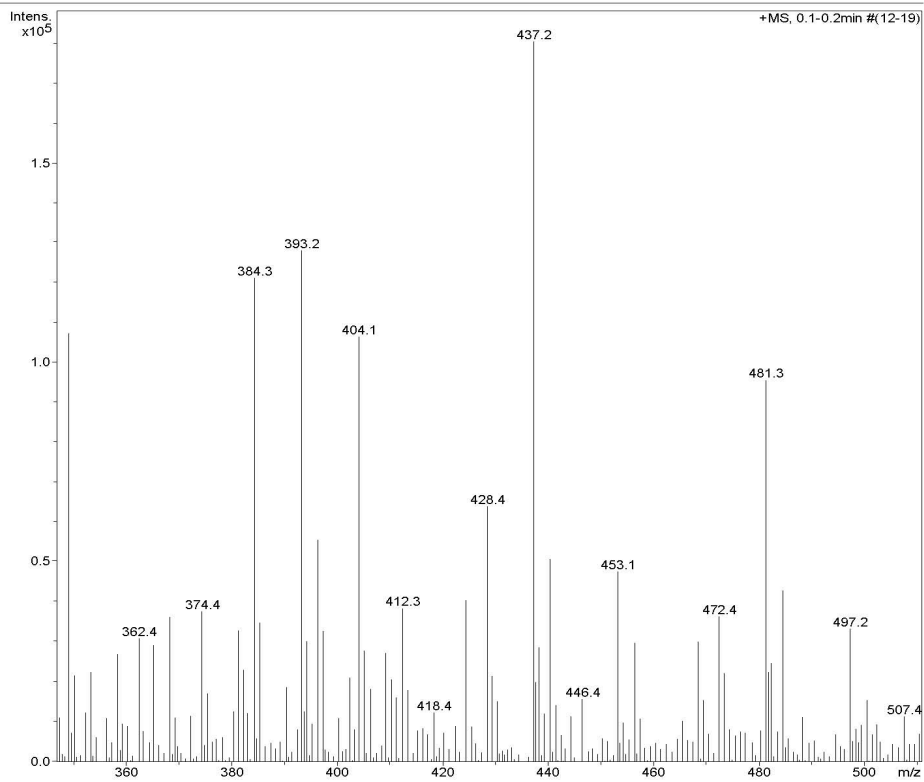
Acquisition Parameter

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Averages 8 Spectra

Positive
100 m/z
n/a

Alternating Ion Polarity off
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Auto MS/MS off

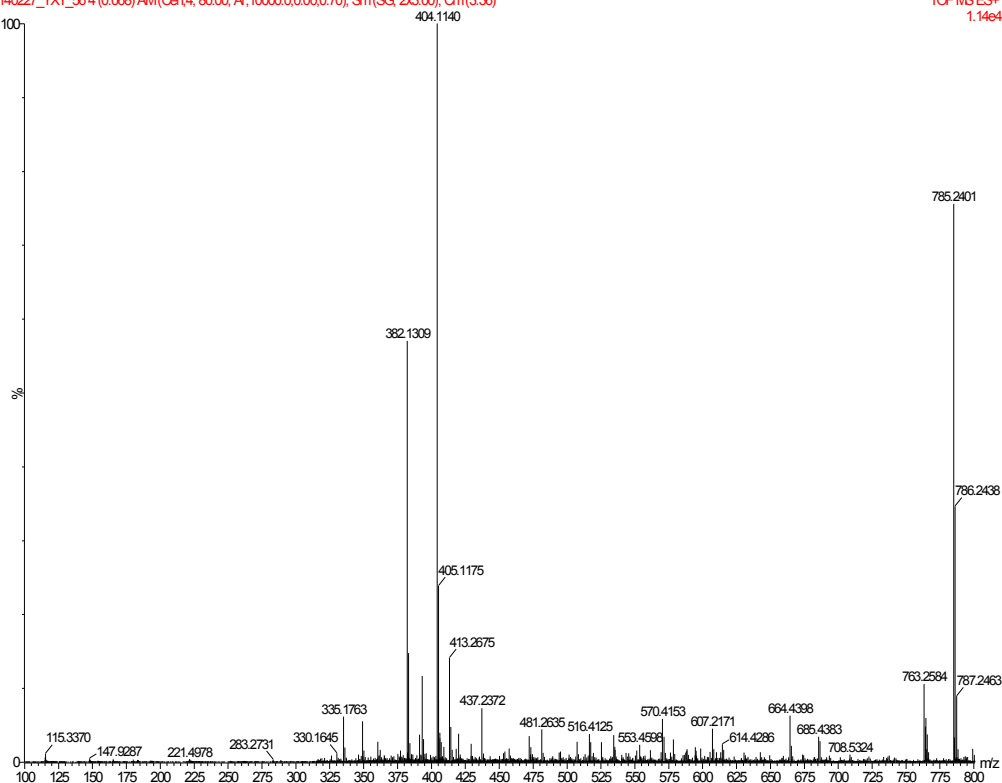


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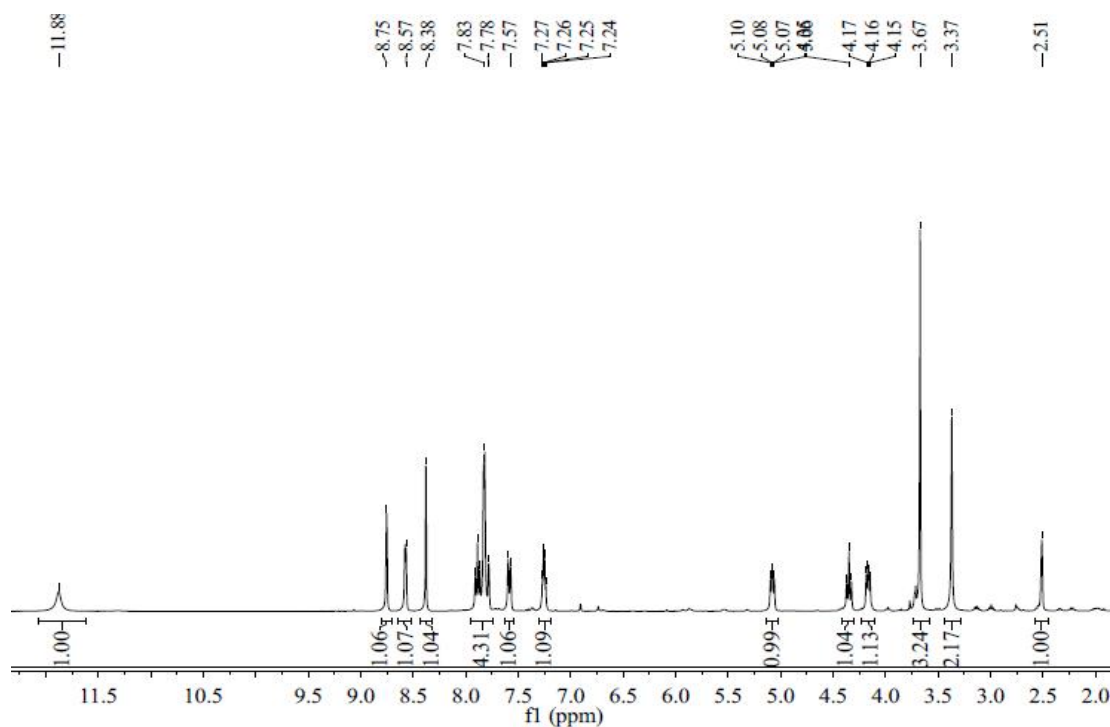
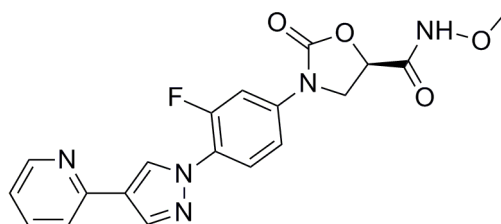
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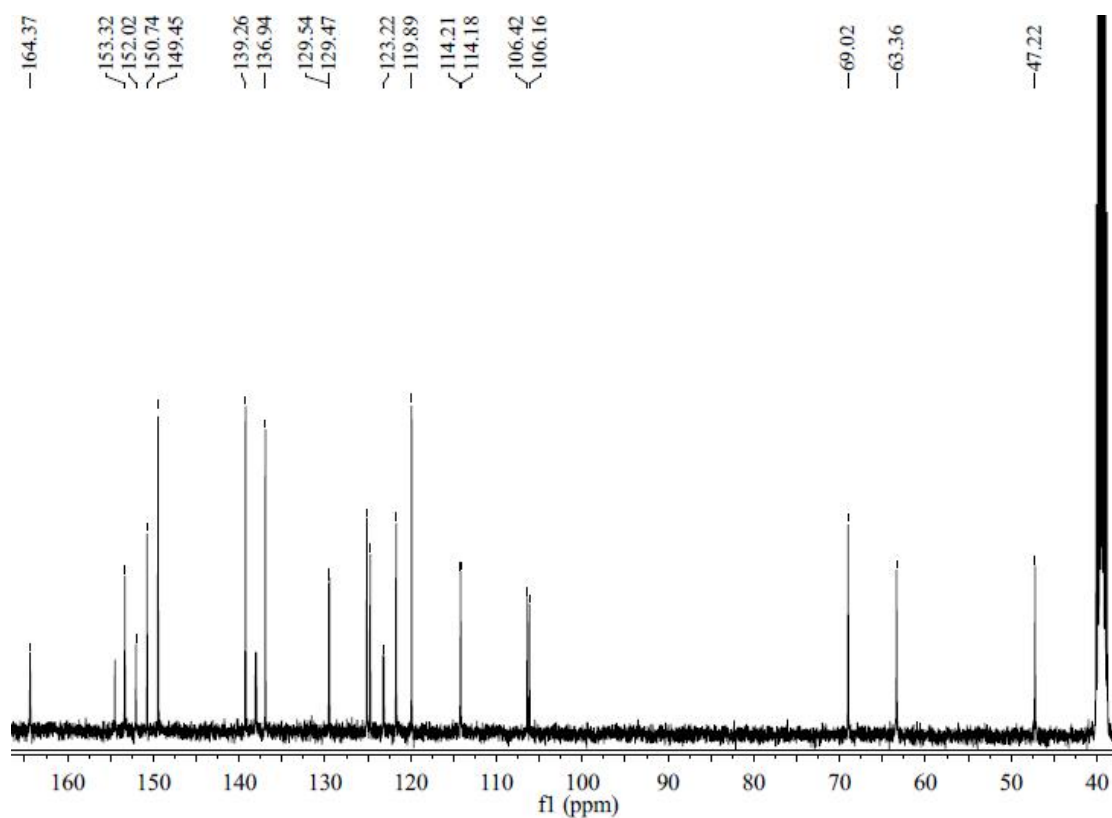
27-Feb-2014

TOF MS ES+
1.14e4



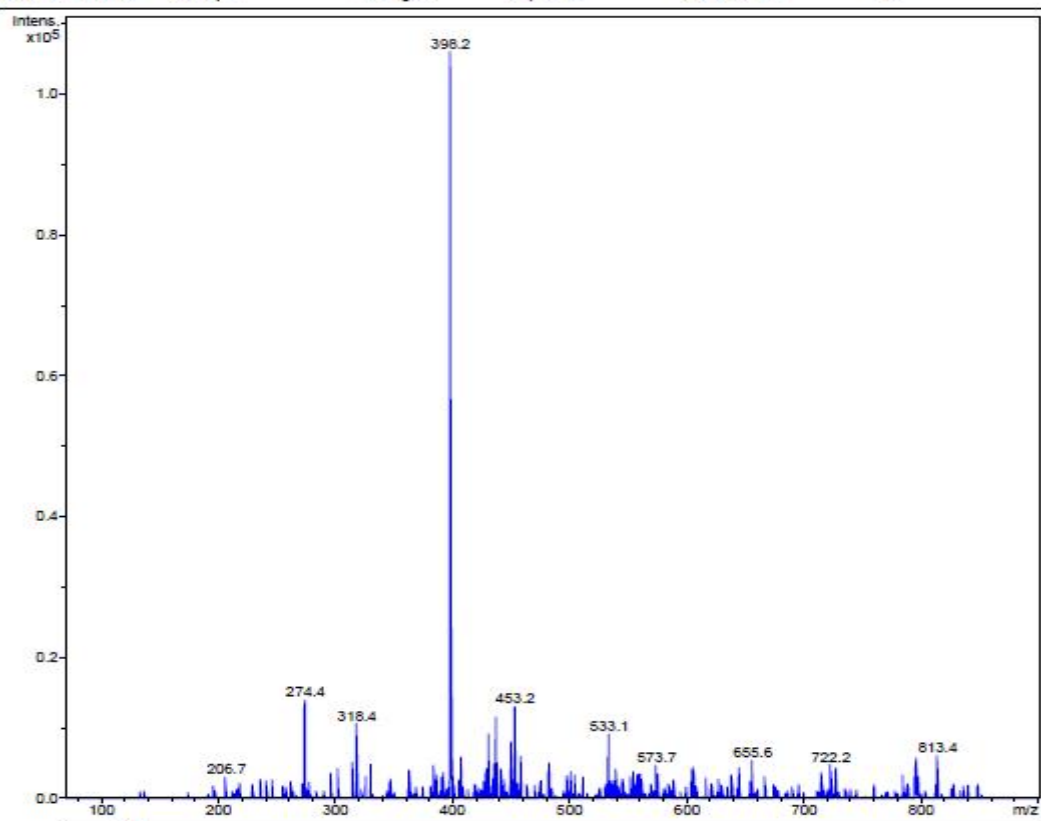
Compounds 45





Acquisition Parameter

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11:17:30

27-Feb-2014

140227_YXY_61 7 (0.120) AM(Cen,4, 80.00, Ar,10000.0,0.00,0.70); Sm(SG,2x3.00); Om(4.36)

TOF MS ES+
3.11e4

